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An Inquiry into the Structure of the Si_{60} Cluster: Analysis of
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by

Daniel A. Jelski, Z. C. Wu and Thomas F. George

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Departments of Chemistry and Physics
State University of New York at Buffalo
Buffalo, New York 14260

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AN INQUIRY INTO THE STRUCTURE OF THE Si_{60} CLUSTER: ANALYSIS OF
FRAGMENTATION DATA

Daniel A. Jelski
Department of Chemistry
State University of New York, College at Fredonia
Fredonia, New York 14063

Z. C. Wu and Thomas F. George
Departments of Chemistry and Physics & Astronomy
239 Fronczak Hall
State University of New York at Buffalo
Buffalo, New York 14260

Abstract

A model is proposed to describe the structure of large, silicon clusters. The model is illustrated for the 60-atom cluster. A structure consisting of stacked, naphthalene-like planes is investigated. Computational evidence is given in support of this hypothesis, and it is shown to be consistent with experimental photofragmentation results.

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I. Introduction

Much experimental data has been accumulated on the properties of large silicon clusters, ranging up to 60 atoms in size. Smalley and coworkers have investigated both the fragmentation patterns^{1,2} and reactivities³ of these clusters. Other authors have dealt with the photofragmentation pattern of smaller clusters.⁴ Recently, an interesting paper has appeared detailing experimental results of the reactivities of silicon clusters with ethylene,⁵ and fragmentation via electron impact studies.⁶

On the theoretical side, much less has been accomplished, especially since there are such a large number of possible structures for large clusters. Tomanek and Schluter (TS)⁷ have used a tight-binding method to calculate the coherence energies for clusters ranging up to 10 atoms in size. These results were compared with calculations using the local density approximation. The two methods are in qualitative agreement, and even quantitative conclusions are probably justified in some cases. Ab initio calculations were performed by Raghavachari et al.⁸ All of these studies refer to clusters with fewer than 12 atoms. Finally, Kupka and Jug⁹ performed interesting calculations on larger clusters by assuming that they consisted of bulk fragments.

While we are primarily interested in larger clusters, a quick review of the discussion surrounding Si_{10} is relevant. Several structures have been proposed. TS initially suggested a close-packed arrangement, a capped octahedron.⁷ Phillips¹⁰ originally suggested an adamantane structure for Si_{10}^+ , arguing that this was closer to the bulk, tetrahedral geometry. But very recently, Chelikowsky and Phillips have proposed the distorted

tetracapped triangular prism as the most likely candidate.¹¹⁻¹³ A similar structure is calculated by Ballone et al.¹³

More recently, Jarrold et al.⁵ have produced evidence to show that at least two isomers of Si_{10} exist. They further state another important point, which constitutes one of the premises of this paper, that cluster reactivity and stability are unrelated. Presumably, stable clusters are formed after long times, whereas the reactivity is a short-time phenomena. A corollary to this statement is the notion that photofragmentation is a form of reactivity. Thus, in what follows, we assume that the fragmentation pattern is primarily a function of the parent cluster rather than the relative stabilities of the daughter clusters. The key to interpreting fragmentation data, therefore, is to investigate the structure of the parent. This assumption is clearly more valid as the parent clusters become larger. For small clusters, approach to equilibrium is a rapid process and probably occurs on a time scale similar to the reactivity. Thus the results of Bloomfield et al for clusters with 11 or fewer atoms probably indicate that Si_6^+ and Si_{10}^+ are stable species. Similar arguments cannot be drawn from the fragmentation pattern of larger parents.

Experimental evidence of reactivities seems to substantiate the above assumption.³ A dramatic variation in the reactivity of silicon clusters with ammonia and methanol, as a function of cluster size, was observed. A periodicity in units of 6 atoms was observed, with Si_{36}^+ and Si_{42}^+ being most reactive, while Si_{39}^+ was less reactive by two orders of magnitude. Clearly, this variation cannot be attributed to cluster stability. Starting with a model proposed by Phillips,¹⁴ we¹⁵ have used the tight-binding method to

from our suggestion, but does seem to indicate that a stacked cylinder is a more appropriate geometry than a bulk fragment.

In this paper, we present a model of medium sized silicon clusters, and we use Si_{60} as an initial example to investigate. Briefly stated, the model is as follows. Small silicon clusters, with less than 12 atoms, are probably molecular in structure. The available evidence seems to indicate that the bulk fragment is not a plausible form for silicon clusters. This is seen most dramatically in the case of Si_{10}^+ , where we can probably exclude the adamantane structure from further consideration. The capped octahedron proposed by TS does seem plausible, especially since it minimizes surface area and dangling bonds, as does the capped prism. As mentioned, the experimental evidence suggests two isomers of Si_{10}^+ exist. However this issue is eventually resolved, we argue that the structure of the stable Si_{10} cluster yields little information about fragmentation pattern of larger species

At the other extreme, bulk silicon is stable in the diamond configuration, of which a 10-atom fragment has an adamantane structure. Each atom is tetra-coordinated, and the orbital structure seems to be a straightforward sp^3 hybridization. This is distinct from the smaller, close-packed, molecular species in which the coordination number can be larger than four.⁵ The issue to be discussed, then, is how do medium-sized clusters arrange themselves between these two extremes. We suggest that a strained, sp^3 hybridization is the most probable configuration. Most atoms in our structures will be tetra-coordinated, with some exceptions.

dangling bonds. The corollary to this statement is the idea that silicon clusters will form graphite-like structures as long as there are no (or few) internal atoms. Internal atoms, unconstrained by surface effects, will "relax" to the bulk, tetrahedral geometry.

The remainder of this paper considers how this model applies to Si_{60} , and investigates its fragmentation pattern. The next section describes the calculations and results, followed by a brief conclusion.

We are interested in the Si_{60} cluster, for reasons that will become apparent. To begin, we review the experimental evidence of interest here.² When Si_{60}^+ is fragmented with an ArF laser, almost all daughter fragments are in the 6-11 atom range. A smaller amount fragments by losing one atom, yielding a Si_{59}^+ cluster. The laser-fluence dependence indicates that this is a two-photon process. Of the smaller fragments, Si_{10}^+ is the most common. The experimenters argue that any charge will tend to form on the larger daughter, and so the absence of any larger clusters probably indicates that they are not formed at all, instead of being neutral and hence undetected. The experimenters report that other clusters also fragment into 10-atom pieces, most notably Si_{20}^+ , for which Si_{10}^+ is almost exclusively the daughter fragment.

We are concentrating on Si_{60}^+ because it is the largest cluster for which any experimental data are available, and since the experimental results are relatively unambiguous. We are interested in size, primarily because our fundamental assumption is most likely to be true for large clusters. Despite the simplicity of the experimental results, however, we are required to make some simplifying assumptions. These are, first, that the positive ion behaves essentially the same as the neutral species, which is reasonable since the addition of one electron in a 240-electron system is probably not significant. We will therefore report data only for the neutral cluster. We have checked our results for positive clusters and found only minor differences in the answer.

Secondly, we will ignore the single-atom fragmentation route since this process does not seem to yield much information about the structure of the

For comparison, we have performed a similar analysis of Si_{60} as a bulk fragment arranged as spherical as possible to minimize surface energy. The coherence energy for this structure is found to be -3.2 eV.

To test the results against the experimental fragmentation data, we have calculated the bond energies, which are reported in Fig. 4. The strongest bonds are those marked "O". This strength is due to the conjugated nature of the rings and the fact that the atoms in this group are no more than tetra-coordinated. The next strongest bonds are those marked "X". These involve atoms with higher coordination numbers, and hence the bonds are weaker. The average value of the 1-6 bond taken alone is 0.137. Finally, the weakest bonds are between the planes. The fragmentation of the cluster into 10-atom pieces is supported by this result.

The explosive nature of the fragmentation is not revealed by the average figures. In Fig. 5 we illustrate the average bond strength connecting each of the layers. It can be seen that the bond strength parallels the charge density distribution. The atoms at each end contribute electrons to their neighbors, and hence the bonds between the extreme planes and those just inside are strong. Similarly, the electron density is small in the center of the molecule, and so the bond between planes 3 and 4 is also strong. The weakest bonds are found between planes 2,3 and 4,5. Thus any fragmentation of the molecule is likely along these lines, and we are left with three, 20-atom fragments.

Despite the fact that Si_{20} as two, stacked planes yields a coherence energy of -3.3 eV, this is not likely to be a stable configuration. The average bond strength between the planes is found to be 0.130. We believe

that Si_{20} thus rapidly dissociates into two Si_{10} clusters. We assume this to be especially true given the large amount of energy in the molecule, the total effect being a two-photon process. It is appropriate to point out that Si_{20}^+ fragments almost exclusively into 10-atom fragments, and this could be described by assuming the di-naphthalene structure. In this event, the complete disappearance of Si_{20}^+ from the Si_{60}^+ fragmentation spectrum can only be accounted for by the excess energy argument, or by invoking the stability of the Si_{10}^+ cluster (in violation of our assumption). While we have not yet investigated the matter closely, we believe that Si_{20} probably consists of two, six-membered rings each with a cap of four atoms.

More obvious is the fact that Si-naphthalene is not a stable form of the Si_{10} cluster. Figure 6 illustrates a possible mechanism by which the naphthalene form can rearrange to the capped octahedron. This involves breaking one bond and the formation of several others.

We have also analyzed the bond strengths of the spherical bulk fragment. In the interior of the sphere, all atoms are tetra-coordinated, and the bond strength should be similar to that of the bulk. For the 20 most interior atoms, the average bond strength is 0.159, where the average is taken over 110 bonds. This compares to the bulk value of 0.117. The next 20 atoms are frequently, but not always, tetra-coordinated. The lower coordination number implies that each bond is stronger, and an average over 90 bonds yields a strength of 0.189. Similarly, the outermost layer contains only 64 bonds, with an average strength of 0.218. Similarly, the bulk has an average bond length of 2.41 Å, whereas in the sphere, bond lengths range from 2.33 Å to 2.42 Å. This is an indication of surface

effects, and the tendency to minimize surface area. Hence atoms are slightly closer together in the cluster compared to the bulk.

The bulk fragment can probably be excluded from further consideration since there is no obvious plane along which to fragment the species. Thus a large number of different sized fragments would be expected, in particular, large fragments with 50 or more atoms. Secondly, there is no unique way to construct such a cluster, and a huge number of isomers would be expected. This, too, would lead to a broadening of the fragmentation spectrum.

III. Conclusion

We believe we have demonstrated the plausibility of our model, at least with respect to Si_{60} . For large clusters, the structure of stacked naphthalene planes is reasonable, whereas for smaller clusters the six-membered rings appear more likely. A problem arises for the smaller clusters in that Si_{10}^+ is also an important part of their fragmentation spectrum. As remarked in the Introduction, the stability of the daughter ions may play a larger role in the fragmentation pattern as clusters get smaller. But this problem remains to be investigated. No experimental evidence exists for the Si_{39}^+ cluster depicted in Fig. 1, but it is difficult to see how a 10-atom fragment is likely.

It is also important to comment on the spectrum dispersion. Clearly, Si_{60} is sufficiently complex that different isomers can occur. It is certainly possible to imagine 6-membered rings stacked 10 high, or 9- or 11-membered rings, or permutations thereof. Each of these would yield a different fragmentation pattern. The fundamental notion, however, is that the clusters consist of stacked, slightly conjugated planes.

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FIGURE CAPTIONS

- Figure 1. Calculated structure of Si_{39}^+ , taken from Ref. 10.
- Figure 2. Proposed structure for the Si_{60} cluster, consisting of six stacked, 10-atom naphthalene-like rings.
- Figure 3. Charge density distribution in Si_{60} . Each line represents one naphthalene plane, and the number is the total charge on that plane, in units of the charge of an electron.
- Figure 4. Average bond strength between different categories of bonds within the proposed Si_{60} cluster. The numbers are unitless.
- Figure 5. Average bond strength of the bonds between each of the planes in the proposed Si_{60} cluster. Each number is an average over 10 bonds. The numbers are unitless.
- Figure 6. Possible sequence of steps in the rearrangement of Si-naphthalene (shown in Fig. 4) to the capped octahedron structure proposed in Ref. 6. (a) illustrates the bending of the rings so that atoms 2, 5, 7 and 10 begin to bond. Also shown is the back-bending of atoms 8 and 9. (b) illustrates the breaking of the bond between 3 and 4, along with the twisting of the caps, yielding the final result shown in (c).

Fig. 2

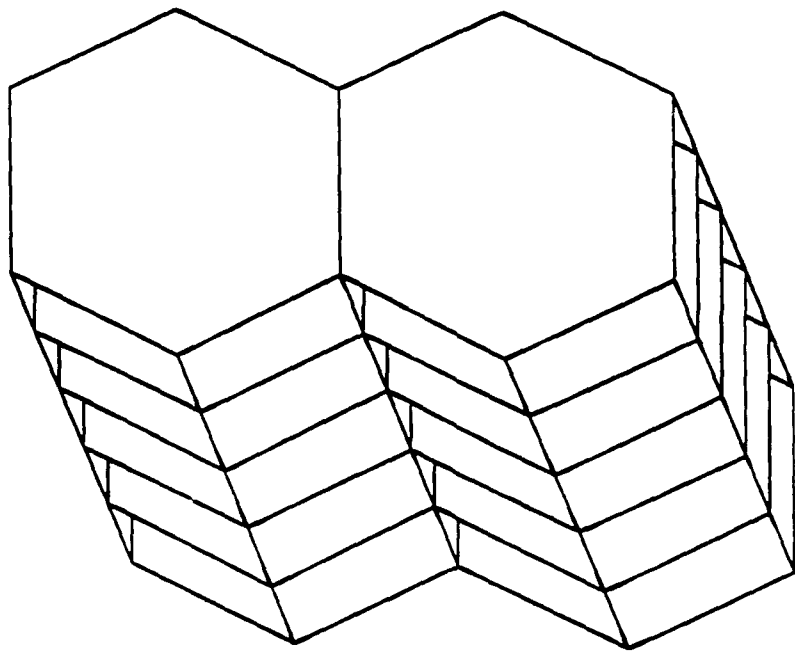
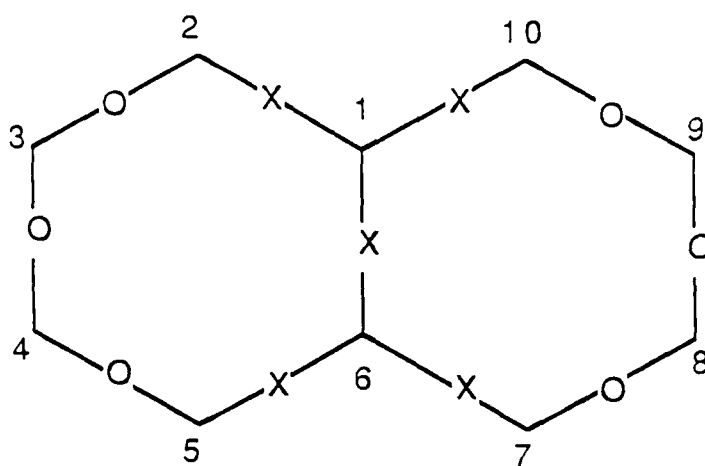


Fig. 4



X - 0.146

O - 0.185

Between Planes - 0.139

Fig 5

0.171

0.104

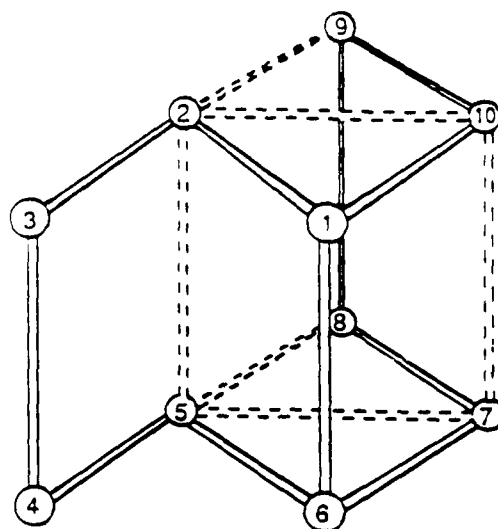
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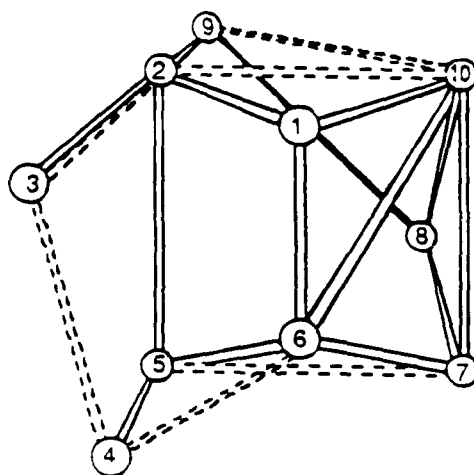
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Fig. 6

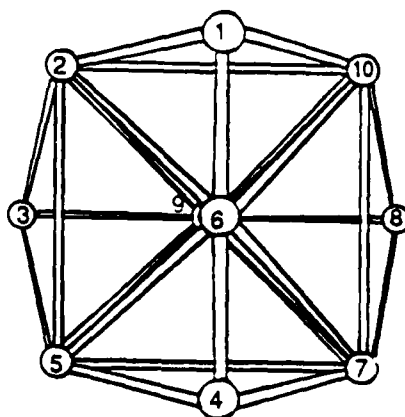
(a)



(b)



(c)



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